Three-dimensional numerical simulation of crystal and crucible rotations during Czochralski growth of Ge$_x$Si$_{1-x}$ single crystals

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Abstract
The influence of crystal and crucible rotations on the flow field and the radial segregation of silicon are predicted during the growth of Ge$_x$Si$_{1-x}$ crystals by the Czochralski method under microgravity conditions. Time-dependent 3-dimensional numerical simulations are carried out to present the influence of several rotation rates on the radial segregation and flow fields during the growth of Ge$_x$Si$_{1-x}$. Thermal and solutal Marangoni convection are also considered during this study. Different crystal rotation rates varying between 0 and 30 rpm and stationary or –2 rpm crucible rotation rates are considered. The results show that the crystal and crucible rotation rates have significant influence on the flow field and radial segregation. It is clear that crystal and crucible rotations with an optimum rotation rate lead to good mixing along the growth interface and result in a crystal with a uniform concentration distribution.

Key Words: Czochralski, Ge$_x$Si$_{1-x}$, Marangoni convection, segregation, surface tension

1. Introduction

Germanium and silicon are used in many applications in electronic devices such as transistors, optical components, radar systems, solar cells, and power generators. The composition of the grown crystals is a significant factor in the determination of the quality of the process in all of these devices. However, obtaining uniform composition during Ge$_x$Si$_{1-x}$ growth is difficult due to the differences in the physical properties of Ge and Si. Convection leads to oscillatory motions in large systems, which result in fluctuations during the crystal growth. If the segregation coefficient $k_s$ is over 1, additives are transferred to the crystal. Segregation, or unbalanced impurity distribution, is due to the fluctuations and unlevelled rate of absorption and the diffusion through the crystal. If the growth of the crystals is carried out in the absence of gravity, uniform dopant distribution can be obtained in Ge$_x$Si$_{1-x}$, as gravity-driven convection is eliminated. On the other hand, the unsteady flow and disturbance in the temperature field can be seen due to surface tension forces. These variations can change the growth velocity and generate microsegregations in the crystal. In addition, the crystal quality can also be affected by the 3-dimensional (3-D) flow in the melt where the segregation takes place. The influence
of Marangoni convection in crystal growth was discussed in many studies [1–6] and it was confirmed that convection due to the variation in surface tension severely affects this process. Therefore, it is clear that a large deviation of the flow fields will be seen if Marangoni convection is ignored. It was also determined that the flow becomes 3-D and oscillatory due to Marangoni convection and leads to segregation.

Segregation in the Czochralski (Cz) growth process was discussed in some studies. The segregation phenomenon in Ge$_x$Si$_{1-x}$ crystal growth was discussed in [7–10]. These experimental studies considered the concentration variation in growth direction, deficiencies in the grown crystal, influence of $k_s$, and the rate of growth. Some 2-D and 3-D numerical studies discussed the segregation in the Cz growth [11,12]. Smirnova et al. [13] demonstrated the severe influence of flow patterns and heat transfer on segregation using a 3-D numerical model. The results of these studies indicated that segregation is due to the convective mass transfer. In [14–16], the relations between convection fluctuations and segregation in the crystal during solidification in the horizontal Bridgman method are studied. The results present the effects of the convection velocity oscillations on the segregation.

The most effective way to achieve flow and thus segregation control is by external forces. These forces are used to decrease the influence of convection in order to suppress the 3-D effects, which in turn cause segregation. The use of magnetic damping and axial heat processing (AHP) are 2 known approaches. The flow intensity decreases with the increasing of the magnetic field strength. There are many studies that discuss the influence of either magnetic field or AHP, such as [17–19]. Crystal growth under the effect of crystal and crucible rotations has been regarded as another way to achieve growth control. First of all, rotating crystal served to ensure the radial symmetry of the thermal distribution, thus ensuring that the crystal grew as a cylinder. Later, it came to be realized that the rotation also helped to ensure the radial uniformity of the distribution of added dopants. In order to stabilize the 3-D flow, the crucible and crystal are generally rotated in opposite directions, where the centrifugal forces counteract the surface tension and buoyancy-driven forces and damp the influence of the 3-D flow. Many studies were carried out to find the effect of crystal and crucible rotation on the flow field during crystal growth. For the sake of brevity, only some of them will be mentioned here and numerical studies will be the main focus. A simple, laminar, axisymmetric 2-D model was used by Li et al. [20] to determine the influences of the crystal and crucible rotations in a small Cz furnace. It was found that the natural convection is suppressed by the rotations of the crystal and crucible. Moreover, the rotations of the crystal and crucible retard heat transfer and increase the temperature difference between the crystal and crucible wall. A set of 3-D numerical simulations with a rotating disk was conducted to find the surface pattern of the melt in a Cz crucible by Jing et al. [21]. It was reported that the disk rotation shows a tendency to weaken the Marangoni effect. Basu et al. [22] carried out 3-D unsteady numerical simulations in order to examine the role of crystal rotation on the 3-D turbulent flow pattern in the Cz growth technique. It was observed that the rate of the crystal rotation has a significant stabilizing effect on convection. In addition to this, it was emphasized that small variations in the rate of the crystal rotation change the structure of the flow pattern. Wagner et al. [23] performed simulations to analyze the effects of crucible and crystal rotations on the flow and thermal fields in the crystal growth process. It was found that the crystal and crucible rotations in opposite directions lead to a complex flow. Counteracting buoyancy and surface tension forces controls the flow. It was also found that increases in the rotation rate of the crystal strongly change the flow structure and increase the temperature fluctuations. Geng et al. [24] created a 2-D model to simulate the combined flow in the melt of the Cz process and found that the crucible rotation has an important role in Cz crystal growth to suppress the flow and decrease the heat transfer rate between the crucible wall and the interface. Kumar et al. [25] carried out 3-D
and time-dependent simulations to investigate the flow in the melt in the presence of buoyant, surface tension, and rotational forces. Szymd et al. [26] carried out 3-D numerical simulations for single crystal growth by the Cz technique. A combined flow of crystal rotation-driven forced convection and buoyancy-driven natural convection were presented. It was concluded that an appropriate crystal rotation rate is required in order to prevent floating particles, which can cause polycrystallization, from attaching to the growing crystal. It was also found that as the forced convection becomes stronger, the dopant distribution in the melt becomes more uniform.

Segregation can also take place due to the solutal Marangoni convection. Therefore, it should also be considered during the evaluation of this process. This study determines the role of crystal and crucible rotations on the thermal and solutal Marangoni convections and analyzes the influence of these convections on the segregation during the growth process of Ge$_x$Si$_{1-x}$ by the Cz technique. A time-dependent 3-D model is generated and a microgravity condition is assumed during the simulations.

2. Numerical model

Figure 1 illustrates the schematic model of the process that is used in this study. Some assumptions are made on the shape and temperature of the boundaries and heat transfer through the boundaries, as discussed in [27,28]. Abbasoglu et al. discussed other parameters and fluid properties in detail and nondimensionalized the governing equations with scale factors. The finite volume method is applied to discretize these equations and different algorithms and iterative solvers are used. Moreover, the grid dependence analysis is done with 3 different mesh distributions, with 50$^r \times 50^z \times 50^\theta$ grids being selected for the simulations in this study [27,28].

The present numerical code is validated by comparing the temperature distribution at the liquid surface with the results of [20] for the case of $Ma_T = 3.34 \times 10^4$ and $Ra_T = 0$ with $Pr = 6.7$ in an annular pool. The results of this study and those in the literature are in good agreement, as shown in Figure 2 [27,28].

![Figure 1. Schematic configuration of the Cz model.](image1)

![Figure 2. Radial distribution of the temperature on the liquid surface with $Ma_T = 66340$ and $A_r = 0.275$ in an annular pool.](image2)
The variation in the melt volume is not considered because the grown crystal height is 0.2 mm during the simulated growth time. The time-stepping is done as in [27,28] and is taken as $5 \times 10^{-5}$. It takes about 25 days for each simulation on a 3.00-GHz Pentium IV computer with a 2-GB random-access memory.

### 3. Results and discussion

The properties of the Ge$_x$Si$_{1-x}$ alloy were obtained from [29–33]. The Table shows the other constants and variables required for the calculations. The crystal pulling velocity is set to 2 mm/h. The rotation speed of crystal $\Omega_{\text{cry}}$ changes from 0 to 30 rpm, and the rotation rate of crucible $\Omega_{\text{cru}}$ is 0 for the motionless case and -2 rpm for the other simulations. The initial conditions of the temperature and velocities are extracted from a steady-state simulation that is carried out for $Ma_T = 375$. The results of the stationary condition at $t = 0.4$ are used as the initial conditions for the rotation simulations. At the beginning of the simulation, the nondimensional concentration is taken as 1.

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<td>Segregation coefficient</td>
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The time-dependent response of the circumferential velocity at the monitoring point is shown in Figures 3a–3d. The monitoring point is found at the free surface in the middle of the outer radius of the crystal and the crucible wall. Simulations are carried out at different crystal and crucible rotation velocities for $Ma_T = 625$ ($\Delta T = 12.5$ K). The corresponding power spectra of the time-varying component of the signal ($V - \overline{V}$), which is calculated by subtracting the instantaneous value from the time average, are presented in Figures 4a–4d. For the stationary crucible and crystal, as the temperature pitch passes over a definite limit, 3-D disorders and small-scale oscillations are seen in the basic flow formation, as in Figure 3a. Periodic oscillations, with a single frequency of 112.30, are observed. At low rotation rates ($\Omega_{\text{cru}} = -2$ rpm and $\Omega_{\text{cry}} = 5$ rpm), the amplitude of
the oscillations increases vigorously, as in Figure 3b. This means that the rotations of the crystal and crucible with these rates provoke a 3-D oscillatory flow and are extremely disturbing for the flow field in the melt. This flow is characterized by 2 significant frequencies and some low frequency oscillations, as in Figure 4b. When the crystal rotation rate is increased to moderate rotation rates ($\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 15$ rpm), a regular periodic oscillating flow with a smaller amplitude of velocity fluctuation is observed, as in Figure 4c. The effect of the crystal rotation is dominant and decreases the azimuthal velocity. At higher rotation rates ($\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 30$ rpm), the oscillations become time-dependent and irregular (Figure 3d). The strong broadband noise in the power spectrum is witnessed in the case of $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 30$ rpm (Figure 4d).

**Figure 3.** The time dependency of the circumferential velocity components at $Ma_T = 625$ for 4 different rotation cases at the monitoring point: a) no rotation, b) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 5$ rpm, c) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 15$ rpm, and d) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 30$ rpm.

**Figure 4.** Power spectral density (PSD) of the circumferential velocity fluctuations at $Ma_T = 625$ for 4 different rotation cases: a) no rotation, b) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 5$ rpm, c) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 15$ rpm, and d) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 30$ rpm.
Figures 5a–5d show studies carried out with the same parameters as in Figure 3, except with a higher Marangoni number, $Ma_T = 1250$. The corresponding power spectrum is presented in Figures 6a–6d. For the stationary crucible and crystal at $Ma_T = 1250$, the flow is irregular and time-dependent, as in Figure 5a. A strong broadband noise is observed in the power spectrum for this simulation. At low rotation rates, the amplitude of the oscillations and the main frequency increase, as shown in Figures 5b and 6b. When the crystal rotation rate is increased to 15 rpm, a more regular oscillating flow with a smaller amplitude of velocity fluctuation is detected, as in Figure 5c. The frequency of the signal also decreases. It is obvious that the azimuthal velocity, which is increased with a rising crucible rotation, decreases with the counter rotation of the crystal when the crystal rotation is more dominant. When the crystal rotation is increased to higher rotation rates, the oscillations become time-dependent and irregular (Figure 5d) and the amplitude of the oscillations decreases more. In this case, many significant frequencies appear in the power spectra (Figure 6d).

**Figure 5.** The time dependency of the circumferential velocity components at $Ma_T = 1250$ for 4 different rotation cases at the monitoring point: a) no rotation, b) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 5$ rpm, c) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 15$ rpm, and d) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 30$ rpm.

**Figure 6.** Power spectral density (PSD) of the circumferential velocity fluctuations at $Ma_T = 1250$ for 4 different rotation cases: a) no rotation, b) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 5$ rpm, c) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 15$ rpm, and d) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 30$ rpm.
Circumferential velocity variations shown in Figures 3 and 5 are compatible with the experimental results of Son et al. [34].

The time-averaged flow patterns are presented for $Ma_T = 625$, $Ma_T = 750$, $Ma_T = 1000$, and $Ma_T = 1250$ in Figures 7a–7d, 8a–8d, 9a–9d, and 10a–10d, respectively. The instantaneous velocity fields in the melt are unsystematic. Thus, to determine the fluctuations in the melt and to analyze the effect of the different rotation rates, the averaged flow pattern through a period is used. This sampling began at about $t = 1.15$. A toroidal cell is created near the free surface as the melt moves from the crucible wall toward the crystal. This vortex, due to surface tension forces, covers nearly all of the melt. A descending flow is found in the center of the crucible, under the crystal and away from the crystal–melt interface. The downward flow at the center moves until it reaches the bottom of the melt and then moves toward the outside, beside the bottom wall. Several small vortices are also observed at the corners and under the crystal. Similar to in Figure 7a, the flow pattern is nearly axisymmetric. At low rotation rates, a radially inward flow due to the crucible rotation is more effective than the outward flow due to the crystal rotation. The weak vortices found at the upper corners disappear and the other vortices under the crystal lose their strength (Figure 7b). As the crystal rotation increases, a more symmetric flow field is observed near the crystal. In addition to these, 2 vortices are observed at the top corners, as in Figures 7c and 7d. This is because the convection, due to the surface tension, and the crucible rotation create a downflow, which is opposed by the upward flow due to the convection driven by the crystal rotation. The strength of this pump-up flow increases with increased crystal rotation. Similar characteristics to those in Figure 7 can be observed in Figure 8. However, the meeting point of the upflows and downflows underneath the crystal moves downwards due to the increased effect of the Marangoni convection. With a further increase of the Marangoni number, $Ma_T = 1000$, the pump-up effect disappears, even for moderate crystal rotation rates, due to a stronger downflow, and the meeting point moves further downwards compared to Figures 7 and 8 for the high rotation rates (Figure 9). These flow structures are also observed in Figure 10, with a difference in the number of vortices being seen just under the crystal.

**Figure 7.** The time-averaged flow fields at $Ma_T = 625$ for 4 different rotation cases: a) no rotation, b) $\Omega_{\text{cru}} = -2$ rpm and $\Omega_{\text{cry}} = 5$ rpm, c) $\Omega_{\text{cru}} = -2$ rpm and $\Omega_{\text{cry}} = 15$ rpm, and d) $\Omega_{\text{cru}} = -2$ rpm and $\Omega_{\text{cry}} = 30$ rpm.
The time-averaged isoconcentration fields are shown in Figures 11a–11d for $Ma_T = 625$. As mentioned above, the nondimensional concentration is equal to 1 all over the melt before solidification. A Si-low region is

Figure 8. The time-averaged flow fields at $Ma_T = 750$ for 4 different rotation cases: a) no rotation, b) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 5$ rpm, c) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 15$ rpm, and d) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 30$ rpm.

Figure 9. The time-averaged flow fields at $Ma_T = 1000$ for 4 different rotation cases: a) no rotation, b) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 5$ rpm, c) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 15$ rpm, and d) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 30$ rpm.
then created under the crystal due to the absorption of the dopants into the crystal. The Si-low melt moves away from the center of the crucible due to the flow driven by the thermocapillary effect. The Si-low region is formed at around $R = 0$ due to the downward flow in the middle. However, the pump-up flow at the bottom region underneath the crystal, due to the crystal rotation, moves the higher Si concentration up to the meeting point of the pump-up flow and the strong downward flow. This concentration distribution is in conformance with the flow pattern given in Figure 7. The Si concentration decreases due to the absorption of the dopants into the Ge. Owing to the changes in the vortices underneath the crystal, as in Figure 7, the concentration boundary layer varies around the axis under the crystal at different rotation speeds (Figure 11).

![Figure 10](image.png)

**Figure 10.** The time-averaged flow fields at $Ma_T = 1250$ for 4 different rotation cases: a) no rotation, b) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 5$ rpm, c) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 15$ rpm, and d) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 30$ rpm.

The time-averaged isoconcentration field at the crystal-melt interface is shown in Figures 12a–12d and 13a–13d for $Ma_T = 625$ and $Ma_T = 1250$, respectively. At the free surface, the Si concentration is uniform for $Ma_T = 625$ when the crystal and crucible are motionless. The dopant moves to the central axis at the interface with a radially inward flow. Moreover, the dopant concentration decreases due to continuous absorption, but weak vortices oppose and stop the decrease in concentration around $R = 0.25$, as in Figure 7a. The amount of Si does not change in the azimuthal direction between $R = 0.25$ and $R = 0.5$ because the isoconcentration lines are concentric. However, the amount of Si changes due to the flow of the small vortices under the crystal around $R < 0.25$. In this region, the concentration pattern is formed from 8 spikes. As the crucible and crystal start rotating, the Si concentration is totally nonuniform for $R < 0.25$ due to the 3-D and oscillatory flow, as in Figure 12b. However, the forced convection becomes dominant due to a further increase in the crystal rotation and uniform distribution is obtained for the moderate and high rotation rates in the vicinity of the crystal (Figures 12c and 12d). For $Ma_T = 1250$, the concentration distribution is nonuniform under the crystal for the stationary and low rotation rates due to the dominant Marangoni convection (Figures 13a and 13b). However, for the moderate and high crystal rotations, while the forced convection dominates the flow, a more uniform concentration distribution is obtained at the crystal growth interface, as in Figures 13c and 13d. Similar results were reported in [26].
Figure 11. The time-averaged isoconcentration lines at $Ma_T = 625$ during 4 different rotation cases: a) no rotation, b) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 5$ rpm, c) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 15$ rpm, and d) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 30$ rpm.

Figure 12. Concentration distribution at the plane of the growth interface at $Ma_T = 625$ during 4 different rotation cases: a) no rotation, b) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 5$ rpm, c) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 15$ rpm, and d) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 30$ rpm.
Figure 13. Concentration distribution at the plane of the growth interface at $Ma_T = 1250$ during 4 different rotation cases: a) no rotation, b) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 5$ rpm, c) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 15$ rpm, and d) $\Omega_{cru} = -2$ rpm and $\Omega_{cry} = 30$ rpm.

The averaged Si concentration is presented in Figures 14 and 15 for $Ma_T = 625$ and $Ma_T = 1250$, respectively. The Si concentration is averaged in a circumferential direction and in time along the crystal–melt interface. The rising fluid nearby the wall takes the melt upwards, where the Marangoni convection-based flow directs the melt to the crystal near the free surface. Therefore, the homogenous and maximum concentration is observed at that region. The crystal is placed at $-0.5 < R < 0.5$. The dopant rich melt moves to the center due to the internal flow near the interface. During this motion, the dopant is immersed in the crystal and the dopant concentration decreases continuously. In the same way, the radially outer vortical flow under the crystal takes the Si-high melt away from the center. In this region, owing to the absorption, the Si amount decreases. The dopant amount is minimal near $R = 0.25$ due to the radially inward and outward flow under the interface for the stationary and low crystal rotation cases, and a W-shaped profile is observed. These are similar characteristics for both $Ma_T = 625$ and $Ma_T = 1250$ (Figures 14 and 15) with the stationary and low rotation rate cases. Owing to the stronger flow, mainly induced by the more dominant crucible rotation and Marangoni convection, the Si concentration in the high concentration region has a short absorption duration while moving under the interface to the lower Si melt in the motionless case and at low rotation rates. This formation decreases the difference between the high and low Si concentration at the interface. However, the counteracting forced convection, due to the crystal rotation, is more effective as the rotation rates increase, and
that leads to an increase in the absorption time due to a decrease in the flow intensity. Thus, the minimum Si concentration is lower for the moderate and high rotation rates. In addition to this, the concentration profile is rather uniform due to the stronger counter rotation that leads to a more symmetric flow field under the crystal, as shown in Figures 7 and 10. Therefore, the following conclusion can be drawn from these results. At low rotation rates, the absorption of the Si concentration is low and its distribution is nonuniform, but at higher rotation rates, the absorption of the Si is high and a more uniform concentration distribution is obtained at the interface.

\[ R_C^{-1} \]

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Figure 14. Radial distribution of the circumferentially and time-averaged Si concentration at \( Ma_T = 625 \) during 4 different rotation cases at the plane of the growth interface.

Figure 15. Radial distribution of the circumferentially and time-averaged Si concentration at \( Ma_T = 1250 \) during 4 different rotation cases at the plane of the growth interface.

Within the crystal growth process, the maximum Si concentration at the crystal–melt interface varies continuously. This change is presented in Figures 16a–16d and 17a–17d for \( Ma_T = 625 \) and \( Ma_T = 1250 \), respectively, where the influence of different rotation rates is also shown. Figures 16a and 17a show the stationary cases. In these cases, as stronger Marangoni convection takes place, the maximum concentration difference decreases due to a lower absorption time, but the amplitude increases. The fluctuation amplitude is weak and the variation is periodic for the stationary case at \( Ma_T = 625 \). The variation becomes smaller as the rotation begins. Interestingly, for both the low and high rotation rates, a chaotic behavior is observed (Figures 16b and 16d) due to the dominant effects of the cooperative forced convection, aided by the crucible, and the Marangoni convection for the low rotation rates and forced convection, aided by the crystal rotation, for the high rotation rates. However, regular and steady variation is obtained with a moderate rotation rate (Figure 16c) due to the effect of the counteracting forced convection. At a higher \( Ma_T \), chaotic behavior is observed due to the higher amplitudes of the fluctuations that lead to the lowering of the maximum concentration difference at the interface (Figure 17a). At low rotation rates, there is no major difference from the stationary case due to strong Marangoni convection that is dominant in the flow, which overcomes the influences of the forced convection shown in Figure 17b. At higher rotation rates, as the counteracting forced convection due to the crystal rotation becomes more effective, both the maximum Si difference at the interface and the amplitude of the fluctuations decrease, but these fluctuations are still exhibiting a chaotic behavior.

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Figure 16. The time variation of the maximum Si concentration difference at the growth interface at $Ma_T = 625$ during 4 different rotation cases: a) no rotation, b) $\Omega_{cru} = -2 \text{ rpm}$ and $\Omega_{cry} = 5 \text{ rpm}$, c) $\Omega_{cru} = -2 \text{ rpm}$ and $\Omega_{cry} = 15 \text{ rpm}$, and d) $\Omega_{cru} = -2 \text{ rpm}$ and $\Omega_{cry} = 30 \text{ rpm}$.

Figure 17. The time variation of the maximum Si concentration difference at the growth interface at $Ma_T = 1250$ during 4 different rotation cases: a) no rotation, b) $\Omega_{cru} = -2 \text{ rpm}$ and $\Omega_{cry} = 5 \text{ rpm}$, c) $\Omega_{cru} = -2 \text{ rpm}$ and $\Omega_{cry} = 15 \text{ rpm}$, and d) $\Omega_{cru} = -2 \text{ rpm}$ and $\Omega_{cry} = 30 \text{ rpm}$.

4. Conclusions

This study examines the influence of the crystal and crucible rotation on the dopant distribution at the interface of the crystal and the melt during the Cz growth of Ge$_x$Si$_{1-x}$. The simulations are 3-D and unsteady. It is assumed that the simulations take place under microgravity. The results show that the crystal and crucible rotations have a stabilizing influence on the Marangoni convection flow, and, in turn, the radial segregation of the Si. Owing to the rotation of the crystal and crucible in different directions, different flow characteristics are observed due to the variation of the dominant driving force.

At low $Ma_T$ numbers (625 and 750), nearly the same profiles are obtained. For these low Marangoni numbers, if the crucible rotation that cooperates with the Marangoni convection is dominant (low rotation
A complex flow takes place. The Si distribution under the crystal is also nonuniform. However, as the counteracting crystal rotation rate increases to moderate values, the flow becomes periodically oscillatory with smaller amplitudes, and it is also nearly symmetric. It was also found that a more uniform Si distribution is obtained at the crystal-melt interface and the maximum Si concentration difference at the crystal–melt interface decreases. When the crystal rotation rate was further increased to a high rotation rate, a time-dependent, irregular, 3-D rotation-driven flow structure was seen, which did not change the maximum difference in the Si concentration but also increased the amplitude of the fluctuations. Therefore, a moderate rotation rate is beneficial in growing uniform crystals for a low Marangoni number.

At higher $Ma_T$ numbers (1000 and 1250) where the Marangoni convection is stronger, the influence of the examined rotation rates is less than in previous cases. In a low rotation case, the counter rotation of the crystal and crucible does not lead to much of a difference in either the flow or concentration fields as compared to the stationary case. As the counteracting crystal rotation rate increases to moderate and high values, the flow intensity decreases, but the 3-D chaotic structure still exists with smaller amplitudes. However, the maximum difference in the dopant concentration decreases due to better mixing. Therefore, higher rotation rates are needed to stabilize the complex flow pattern and improve the quality of the grown crystal at higher $Ma_T$ numbers.

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References


